

# Laboratory Density Functionals

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## Abstract

We compare several definitions of the density of a self-bound system, such as a nucleus, in relation with its center-of-mass zero-point motion. A trivial deconvolution relates the internal density to the density defined in the laboratory frame. This result is useful for the practical definition of density functionals.

Recently [1], Engel pointed out that the usual form of nuclear Hamiltonians,

$$H = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i>j=1}^A v_{ij}, \quad (1)$$

forbids a proper definition of the nuclear density. Indeed, the center of mass (CM) of the system delocalizes in a plane wave; the nucleus is everywhere, the density is flat. The conclusion holds whether the two-body interaction  $v$  is local or non local and still holds if three-body forces are also present in  $H$ , as long as any explicit density dependence is avoided; Galilean invariance must be ensured.

An elementary modification of  $H$ ,

$$\mathcal{H} = H + A\omega^2 R^2/2, \quad R = A^{-1} \sum_i r_i, \quad (2)$$

traps the CM. The ground state of  $\mathcal{H}$  now factorizes as a product of a Gaussian for this CM and an “internal” wave function of the  $(A-1)$  Jacobi coordinates,

$$\Psi(r_1, r_2, \dots, r_A) = \Gamma(R) \psi_{int}(\xi_1, \xi_2, \dots, \xi_{A-1}),$$

$$\xi_1 = r_2 - r_1, \xi_2 = r_3 - \frac{r_2 + r_1}{2}, \dots, \xi_{A-1} = r_A - \frac{r_{A-1} + r_{A-2} + \dots + r_1}{A-1}. \quad (3)$$

Calculations in the  $\{r_i\}$  representation are much more convenient than those in the  $\{R, \xi_j\}$  one, for obvious symmetrization reasons. The laboratory density,

$$\rho(r) = A \int dr_1 dr_2 \dots dr_{A-1} |\Psi(r_1, r_2, \dots, r_{A-1}, r)|^2, \quad (4)$$

is much easier to calculate than the “internal” density,

$$\sigma(\xi) = A \int d\xi_1 d\xi_2 \dots d\xi_{A-2} |\psi_{int}(\xi_1, \xi_2, \dots, \xi_{A-2}, \xi)|^2, \quad (5)$$

Throughout this note, we shall use the word “internal” instead of “intrinsic” when we refer to properties independent from the CM. This is because we retain the word “intrinsic” for those states out of which rotation bands and/or parity vibrations are modeled. Our understanding is that the adjectives “internal” and “intrinsic” belong to completely distinct concepts and models.

Three remarks are in order at this stage,

i) The density of interest for a density functional theory (DFT) is  $\rho$ , not  $\sigma$ . Indeed the Hohenberg-Kohn theorem derives from embedding the system in an external field, namely replacing  $\mathcal{H}$  by

$$\mathcal{K} = \mathcal{H} + \sum_{i=1}^A u(r_i), \quad (6)$$

then considering the density  $\tau(r)$  of the ground state  $\Xi$  of  $\mathcal{K}$ ,

$$\tau(r) = A \int dr_1 dr_2 \dots dr_{A-1} |\Xi(r_1, r_2, \dots, r_{A-1}, r)|^2, \quad (7)$$

and finally proving that there is a one-to-one map between  $u$  and  $\tau$ . The ground state energy of  $\mathcal{K}$  receives the contribution  $\int dr u(r) \tau(r)$ , out of which  $u$  and  $\tau$  are recognized as conjugate Legendre coordinates, hence the functional Legendre transform which defines the density functional. When  $u$  vanishes,  $\rho$  is that limit of  $\tau$  which minimizes the functional. It seems obviously very difficult to set any similar chain of arguments in the Jacobi representation!

ii) Despite this priority of  $\rho$  for a DFT, the internal nature of  $\sigma$  is compelling for a physical interpretation. It is tempting to calculate  $\sigma$  in the  $\{r_i\}$  representation. With the Gaussian  $\Gamma$  square normalized to unity, one finds

$$\begin{aligned} A^{-1} \sigma(\xi) &= \int dR d\xi_1 d\xi_2 \dots d\xi_{A-2} [\Gamma(R)]^2 |\psi_{int}(\xi_1, \xi_2, \dots, \xi_{A-2}, \xi)|^2 = \\ &= \int dR d\xi_1 \dots d\xi_{A-2} d\xi_{A-1} \delta(\xi_{A-1} - \xi) [\Gamma(R)]^2 |\psi_{int}(\xi_1, \xi_2, \dots, \xi_{A-2}, \xi_{A-1})|^2 = \\ &= \int dr_1 \dots dr_{A-1} dr_A \delta\left(r_A - \frac{r_1 + r_2 + \dots + r_{A-1}}{A-1} - \xi\right) |\Psi(r_1, r_2, \dots, r_A)|^2. \end{aligned} \quad (8)$$

iii) the last Jacobi coordinate also reads

$$\xi_{A-1} = \frac{A r_A - (r_1 + r_2 + \dots + r_{A-1} + r_A)}{A-1} = \frac{A}{A-1} (r_A - R). \quad (9)$$

The density  $\sigma$  therefore also represents, except for a trivial rescaling factor, the density referring to the internal degree of freedom,  $r_A - R$ .

Finally, according to Eqs. (4) and (9), the density  $\rho$  reads,

$$\begin{aligned}
A^{-1} \rho(r) &= \int dr_1 dr_2 \dots dr_{A-1} dr_A \delta(r_A - r) |\Psi(r_1, r_2, \dots, r_{A-1}, r_A)|^2 = \\
&\int dR d\xi_1 \dots d\xi_{A-1} \delta\left(R + \frac{A-1}{A} \xi_{A-1} - r\right) [\Gamma(R)]^2 |\psi_{int}(\xi_1, \dots, \xi_{A-2}, \xi_{A-1})|^2 = \\
&\int dR d\xi_1 \dots d\xi_{A-2} [\Gamma(R)]^2 \left| \psi_{int}\left[\xi_1, \dots, \xi_{A-2}, \frac{A}{A-1}(r - R)\right] \right|^2 = \\
&A^{-1} \int dR [\Gamma(R)]^2 \sigma\left[\frac{A}{A-1}(r - R)\right]. \tag{10}
\end{aligned}$$

The convolution transforming  $\sigma$  into  $\rho$  is transparent, with again an inessential rescaling factor  $A/(A-1)$ . The zero-point motion of the CM blurs the internal density in a way which can be easily inverted, via a deconvolution. The bottom line is,  $\rho$  contains the same information as  $\sigma$ . It is thus possible, and likely much easier, to design a DFT with laboratory densities  $\tau$ . At the end one recovers the internal  $\sigma$  by a deconvolution of  $\rho$ , that solution obtained by the minimization, with respect to  $\tau$ , of such a “laboratory Hohenberg-Kohn functional”.

It will be noticed that the presence in  $\mathcal{K}$  of external potentials  $u(r_i)$  couples the CM degree of freedom  $R$  and the internal ones  $\xi_j$ . There is, in general, no CM factorization for eigenstates of  $\mathcal{K}$ . The factorization occurs at the limit  $u = 0$ . Then one must verify that the *Fourier transform* of  $\rho$  shows the factorized, Gaussian decay at large momenta, implied by the convolution, Eq. (10). Otherwise, deconvolution will fail. This “deconvolution syndrome” is very well documented in the literature about generator coordinates. For the DFT, expansions of the density in harmonic oscillator functions and related polynomials, constrained [2] to satisfy matter conservation, make a useful precaution to avoid the deconvolution syndrome.

For atoms and molecules, CM traps factorizing other wave packets  $\Gamma$  than Gaussians might be convenient, but the link between  $\sigma$  and  $\rho$  remains the same.

We conclude by claiming that a density functional theory for self-bound systems is available with densities in the *laboratory* system, without any loss of information about the internal, physical density.

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## References

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